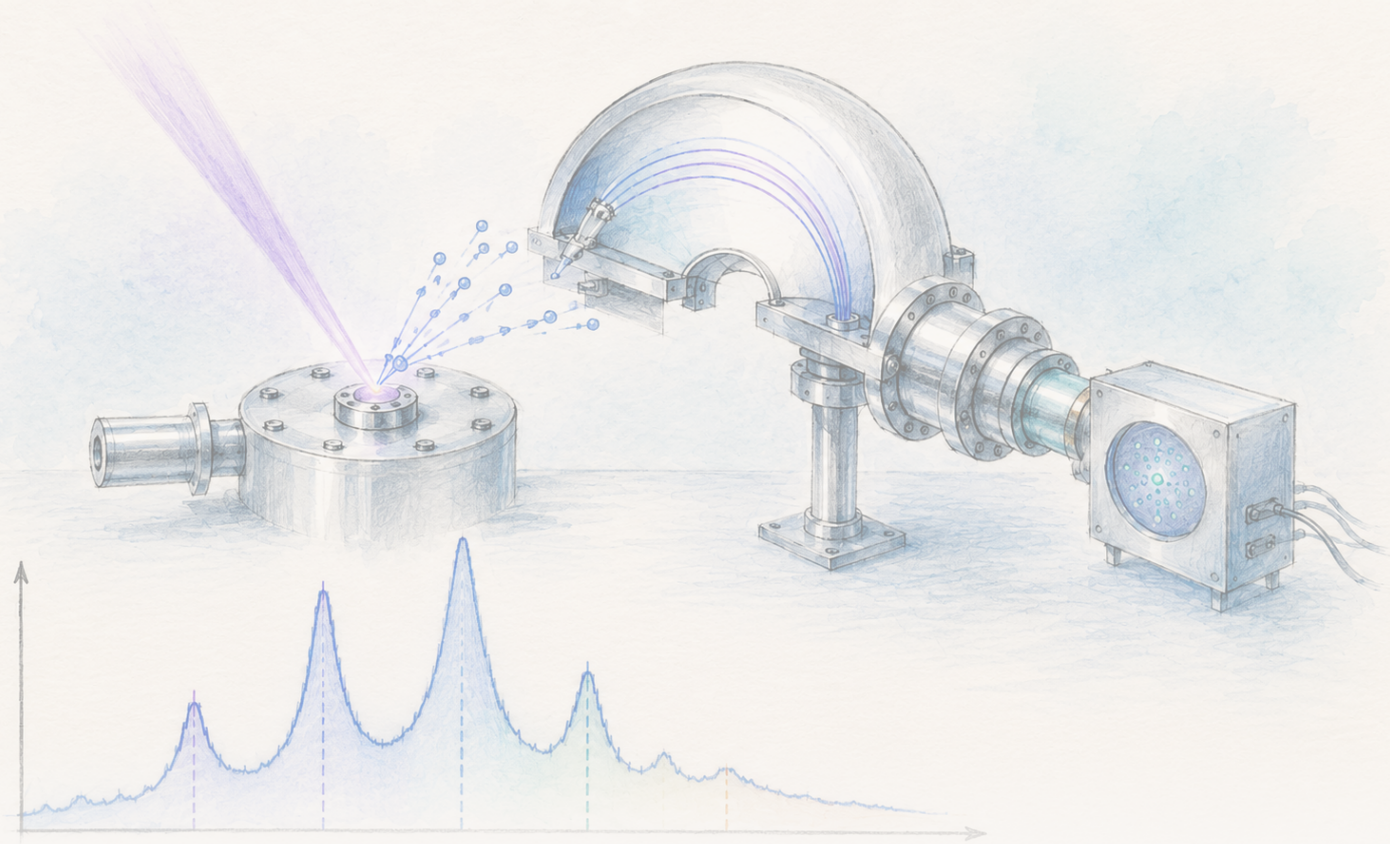


The Clean Paper

WHAT THE PAPER SAYS · WHAT IT DOESN'T · WHY IT MATTERS

Carbon-bismuth triple bond textbook sigma-fi-pi picture eessa hojii dhaabu agarsiisa

Qorannoon Science molecular ion CBi-, heavy-element cousin species triple-bonded beekamoo, cryogenic photoelectron spectroscopy fi relativistic quantum calculations'n qore. Bu'aan strong spin-orbit coupling classical sigma fi pi bonding framework gara relativistic Kramers pairs total angular momentum'n labelled ta'anitti qindeessuu danda'a jechuun direct evidence dha. Ordinary chemical bonding dogoggora hin godhu; heavy atoms baay'ee ulfaataa bira bookkeeping maaliif jijjiiramu agarsiisa.

Written by Matteo · Cross-checked by Vera Rubin · Edited by Michele Renda · Figures by Nova Vela · AI-assisted, human-reviewed

Paper: *Relativistic collapse of the classical triple bond in the CBi- molecular ion*, Deniz Kahraman, Jie Hui, Xin-Yu Zhang, Neil A. Ellis, Hyun Wook Choi, Kirk A. Peterson and Lai-Sheng Wang, Science 393, 184-187 (2026) · DOI: 10.1126/science.aei1285

Triple bond yeroo baay'ee sirrii fi qulqulluu fakkaata. Bismuth garuu akka salphaatti hin qindaa'u.

Boca textbook triple bond keessatti **sigma bond tokko fi pi bonds lama** jiru. Sigma bond kutaa head-on dha; elektiroonii density sarara atoms lama gidduu irratti argama. Pi bond kutaa side-on dha; elektiroonii density sarara sana gubbaa fi jala, yookaan naannoo isaa, argama. Textbook keessatti sigma tokko + pi lama package qulqulluu tokko uuma.

Suuraan kun salphaa dha; atoms salphaa irratti sababaan salphaa ta'a: electrons orbitals bifa isaanii fi spin isaanii conceptually adda ta'ee ibsamuu danda'an keessatti jiraatu.

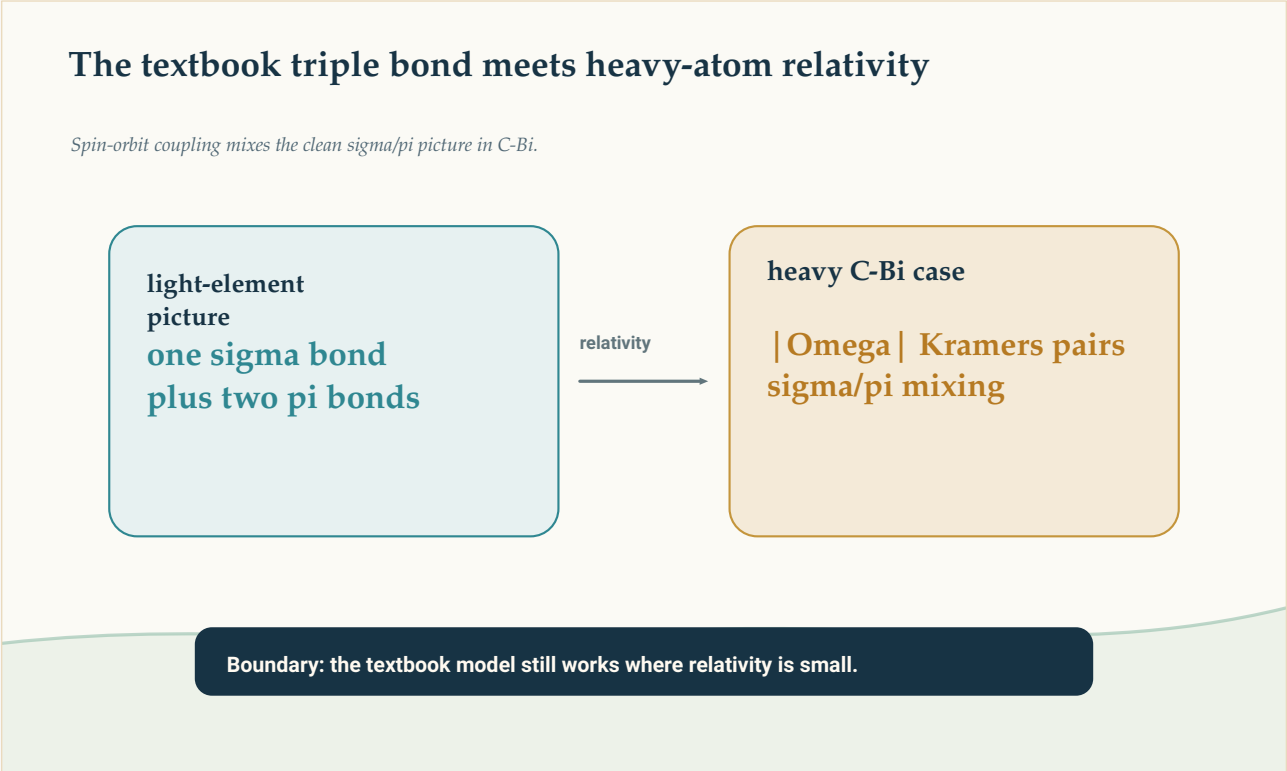
Boca kun soba miti. Periodic table kutaa textbook fakkeenyonni baay'een keessa jiran keessatti approximation baay'ee gaarii dha.

Bismuth kutaa sana miti.

Bismuth protons 83 qaba. Nucleus akkanaa ulfaataa bira, relativity correction xixiqqoo ta'uu dhiisee chemistry keessaa kutaa ta'a. Electrons damee cimaa keessatti socho'u; **spin-orbit coupling** — spin elektiroonii fi orbiitii motion isaa gidduu coupling — organizing fact ijoo ta'uu danda'a. Yeroo kana labels durii namni tokko dagateef hin badne; labels gaarii ta'uu dhiisu.

Barruu Saayinsii haaraan, Deniz Kahraman, Jie Hui, Xin-Yu Zhang, Neil A. Ellis, Hyun Wook Choi, Kirk A. Peterson fi Lai-Sheng Wang irraa, haala qajeelaa tokko qore: molekiyuulii ion carbon-bismuth **CBi-**. Inni CN-, light-element triple-bond sirna beekamaa, waliin isovalent dha. Garuu nitrogen bakka bismuth kaa'uun electron-counting rakkoo sanuma relativistic environment baay'ee ulfaataa keessa galcha.

Bu'aan qulqulluun "triple bonds dogoggora dha" miti. Caalaatti dhiphaa fi nama hawwatu: CBi- keessatti kilaasikaalaa sigma + pi lama description, **relativistic Kramers pairs** total angular-momentum projection'n labelled ta'an keessatti deebisee qindaa'a. Bond sun jira. Bookkeeping durii dha kan kufu.



Light-element triple bond sigma tokko + pi orbitals lama; heavy C–Bi keessatti spin-orbit coupling isa gara |Omega| Kramers pairs sigma/pi mixing qabanitti qindeessa. Bond sun jira — textbook labels qofa hojii isaanii dhaabu.

Original diagram — The Clean Paper CC BY 4.0

Barreessitoonni maal safaran

Barreessitoonni CBi- molekiyuulii beam keessatti bismuth/graphite galma leezerii ablation'n uuman; achiis anion sana high-resolution cryogenic photoelectron spectroscopy fi photoelectron imaging'n qoran. **Anion** jechuun ion charge negaatiivii qabu; as CBi- molekiyuulii carbon-bismuth elektiroonii dabalataa tokko qabu.

Photoelectron spectroscopy yaada salphaa tokko technique rakkisaa keessatti hojjeta. Photon tokko anion irraa elektiroonii tokko baasa. Elektiroonii ba'e anniisaa isaa safaruun elektiroonii balleessuuf anniisaa hammam akka barbaachise, fi neutral electronic haala kam akka ga'ame, hima. Neutral electronic haala jechuun elektiroonii dabalataa erga ba'ee booda electrons hafan qindaa'ina eeyyamame tokko. Photoelectron imaging angular odeeffannoo illee kenna: electrons kallattii kamiin ba'an akkaataa isaanii galmeessa; kun orbiitii elektiroonii eessaa akka dhufe adda baasuuf gargaara.

[video pending]

Animation barnootaa gabaabaa photoemission dhiibbaa: ifa dhufu maateriyaalii irraa electrons baasa, elektiroonii energies haalawwan hafan irratti odeeffannoo kenna — principle sanuma photoelectron

spectroscopy as fayyadame. Waliigalaa technique agarsiisa, CBi- yaalii mataa isaa miti. Biraawzaroota adda addaa irratti akka hojjetuuf The Clean Paper viidiyoo kana gara MP4tti jijjiire; qabiyyeen isaa hin jijjiiramne.

Ijoo speektrumii 4.661 eV irratti electronic bands sadii, **X, A fi B**, agarsiise. Molekiyuulii spectroscopy keessatti X yeroo baay'ee ground electronic haala — neutral molekiyuulii haala anniisaa gadi-aanaa — agarsiisa; A fi B excited electronic haalawwan itti aanan. Higher-energy speektrumii 6.424 eV irratti amaloota dabalataa hin argamne.

High-resolution safartuuwwan adiabatic detachment energies kana kennan:

- **2.3429 eV** X haala'f, jechuun elektiroonii affinity neutral CBi;
- **2.5812 eV** A haala'f;
- **3.5246 eV** B haala'f.

Yaalii shakkii gabaafame electronic energies irratti naannoo **0.0010 eV**, vibrational frequencies irratti **8 cm-1** dha.

Vibrational frequencies safarame:

- X: **681 cm-1**;
- A: **606 cm-1**;
- B: **633 cm-1**.

Lakkoofsi kun haala tokko tokko keessatti bonding irratti odeeffannoo kenna. Bond gabaabaa fi cimaa yeroo baay'ee stretching frequency ol'aanaa qaba; bond dadhabaa yookaan dheeraa frequency gadi-aanaa qaba. Chemistry yeroo hunda caveat malee seera kana hin eeyyamu, garuu handle jalqabaa gaarii dha.

Boca durii eessa rakkoo qaba

Nonrelativistic picture keessatti CBi- akka CN- cousin ulfaataa fakkaata. Filled sigma orbiitii fi filled pi orbitals lama eegda. Elektiroonii tokko baasuudhaan neutral haalawwan usual sigma/pi afaan keessatti assign gochuun danda'ama jedhamee eegama.

Safartuuwwan garuu akkas qulqulluu miti.

Angular distributions rakkoo jalqabaa dha. Detector elektiroonii anniisaa qofa miti, electrons kallattii kamiin ba'an illee safara. Akkaataa sun anisotropy paaraameetira **beta** jedhamee cuunfama. X band beta **1.86** qaba; barreessitoonni dominant p-wave detachment sigma-type orbiitii irraa jedhu. A fi B beta **-0.73** fi **-0.67** qabu, pi-like detachment waliin wal-simu.

Hanga kanaatti manageable fakkaata: X sigma-like, A fi B pi-like.

Garuu vibrational caasaa assignment sanuma dida. Elektiroonii yeroo ba'u molekiyuulii vibrating ta'ee hafuu danda'a; vibration peaks akkaataa **Franck-Condon progression** jedhama. X fi B progressions gabaabaa wal fakkaataa qabu; A ammoo dheerata. A fi B idilee pi-hole haala tokko spin-orbit

kutaalee lama qofa ta'an, bond-length jijjiiramoota isaanii caalaatti wal fakkaachuu qabu. Garuu B karaa tokkoon X fakkaata, karaa biraan A fakkaata.

Contradiction akkasii diagram jalatti dhoksuun salphaa dha. Barreessitoonni faallaa isaa godhu: diagram sun object sirrii ta'uu dhiisuu isaa clue godhu.

Relativistic description

Heavy atoms irratti spin fi orbiitii motion qulqullinaan adda hin baafaman. Hanga caalaatti conserved ta'e projection total electronic angular momentum molekiyuulii axis irratti dha. barruun kana **omega** jedhanii label godha.

Kun basis description jijjiira. Triple bond sigma tokko + pi lama, spin booda itti dabalu jechuun osoo hin taane, barreessitoonni haalawwan relevant **relativistic Kramers pairs** ta'anii ibsu. Kramers pair jechuun spinors degenerate lama time-reversal symmetry'n sirnoota odd-number electrons qabu keessatti barbaachisan. Jechi teknikaa dha, qabxii garuu salphaa: relativistic haala keessatti one-electron objects natural **spinors** dha, idilee spin-free orbitals irratti spin booda maxxansamu miti.

Guutummaatti relativistic shallaggii pure pi-like **|omega| = 3/2** Kramers pair tokko, fi **|omega| = 1/2** Kramers pairs lama substantial sigma/pi mixing qaban kenna. Afaan salphaan, pair tokko ammas pi kutaa fakkaata; lamaan biroo sigma yookaan pi qulqulluu ta'anii hin hafan. "Collapse" title barruu keessaa kana: bonding baduu miti; **kilaasikaalaa sigma/pi separation afaan sirrii ta'uu dhaabuu** dha.

Computations decoration miti. Barreessitoonni four-component Dirac-Coulomb coupled-cluster malleen, including DC-CCSD(T) ground fi low-lying haalawwan, fi EOM-IP-CCSD B haala'f, fayyadaman. Calculated C-Bi bond length CBi- keessatti **2.022 angstroms**, anion stretching frequency computed **695 cm-1**, yaalii safartuu waliin dhihoo. Calculated adiabatic detachment energies X fi A safarame waliin dhihoo fi relativistic assignment deeggaru.

B haala shallaggii keessatti delicate ta'ee hafa. Calculated vibrational frequency yaalii waliin xiqqoo dadhabaa wal-sima; barreessitoonni frequency kun degree mixing X fi B haalawwan gidduu jiru irratti baay'ee sensitive ta'uu mallattoo jedhu. Cimaa |omega| = 1/2 mixing sun B frequency A caalaa ol'aanaa gochuufis gargaara. Barruun qulqulluun barruu irraa caalaatti "ifaa" fakkeessuu hin qabu.

Kun maal hin mirkaneessu

- Idilee sigma fi pi bonding faayidaa hin qabu jechuu **miti**.
- Carbon-nitrogen triple bonds, alkynes yookaan light-element textbook fakkeenyonni baay'een redraw godhamuu qabu jechuu miti.
- Heavy-element bond hundi CBi- fakkaata jechuu hin mirkaneessu.
- C-Bi bond hedduu bond miti jechuu hin jedhu.
- Relativistic quantum chemistry optional flourish godha jechuu miti; haala kana keessatti assign-

ment sirriif required dha.
- Maateriyaalii haaraa yookaan chemical technology haaraa ofumaan hin uumu.

Daangaa'n qabxii dha. Kilaasikaalaa bonding afaan yaadota bu'uuraa isaa gara dhugaa ta'an keessatti baay'ee gaarii hojjeta. CBi- faayidaa qabu dha, sababni isaas yaadota bu'uuraa sun hanga kufaatii mul'ataa ta'utti strain ta'u.

Ragaan hammam cimaa dha?

Assignment barreessitoonni godhan irratti ragaa cimaa dha.

Experimentally, barruun high-resolution cryogenic speektra, vibrational caasaa fi photoelectron angular distributions walitti makata. Isaan complementary constraints dha: anniisaa spacings qofti dadhabaa; angular distributions qoftis dadhabaa; tension isaanii gidduu jiru exactly relativistic hiika irratti akeeka.

Computationally, barreessitoonni guutummaatti relativistic four-component malleen fayyadamu, nonrelativistic shallaggii booda spin-orbit coupling correction xixiqqoo ta'ee dabaluu miti. Kun barbaachisaa dha, claimichi spin-orbit coupling molekiyuulii kana keessatti xixiqqoo **miti** jechuu waan ta'eef.

Match perfect miti. B-state vibrational frequency loose end beekamaa dha. barruun molekiyuulii ion tokko qofa qore, chemical addunyaa guutuu miti. Garuu madaallii wabii heavy-element relativistic bonding ta'een CBi- baay'ee ifaa dha: xinnaa, experimentally resolved fi theoretically tractable.

Maaliif barbaachisaa dha

Chemistry bonding suuraan barsiisa. Kun dadhabina miti. Suuraan gaariin quantum makaanikaa waan namaan itti fayyadamu danda'u keessatti compress godha.

Garuu suuraa hundaaf jurisdiction jira. Sigma/pi triple-bond picture haala spin-orbit coupling secondary ta'ee treat godhamuu danda'u keessatti hojjeta. Heavy elements haala sana keessaa bahuu danda'u. CBi- molekiyuulii xiqqaa keessatti exit sana safartuu fi shallaggii bal'ina ibsaa waliin agarsiisa.

Heavy-element chemistry'f kun barbaachisaa dha, sababni isaas bismuth fi neighbors isaa quantum makaanikaa keessatti curiosities exotic miti. Relativistic dhiibbaawwan bookkeeping chemistry idilee keessaa kutaa dha. Heavy atoms bira bonding qophii, interpret yookaan tilmaamuuf hangawwan sirrii conserved ta'an eegu afaan barbaachisa.

Gatiin paperichaa picture durii gowwaa fakkeessuu miti. Wanta caalaatti faayidaa qabu godha: **picture durii eessa load baachuu dhaabu** sirriitti agarsiisa.

Cuunfaa gabaabaa

Kahraman, Hui, Zhang, Ellis, Choi, Peterson fi Wang molekiyuulii ion CBi- high-resolution cryogenic photoelectron spectroscopy fi photoelectron imaging'n safaran; achiis speektra guutummaatti relativistic Dirac-Coulomb coupled-cluster shallaggiiwwan waliin wal-bira qaban. Neutral CBi haalawwan sadii adiabatic detachment energies 2.3429, 2.5812 fi 3.5246 eV qaban argatan. Speektra fi angular distributions salphaa nonrelativistic sigma + pi lama triple-bond picture waliin hin simne. Cimaa spin-orbit coupling bonding gara relativistic Kramers pairs qindeessa: pi-like |omega| = 3/2 pair tokko fi |omega| = 1/2 pairs lama sigma/pi mixing qaban. Kun heavy-element triple-bond sirna keessatti textbook orbiitii labels afaan conserved gaarii ta'uu akka dhaaban kallattii ragaa dha. Idilee chemical bonding reject gochuu miti; bakka tokko relativity bookkeeping fudhatu sirriitti kaartaa godha.

Maddoota

Kahraman, Hui, Zhang, Ellis, Choi, Peterson and Wang, Relativistic collapse of the classical triple bond in the CBi- molecular ion, Science 393, 184-187 (2026)
https://doi.org/10.1126/science.aei1285

Kahraman et al., Tabular Data and Computational Details for the CBi Spectroscopic Analysis, Zenodo (2026)
https://doi.org/10.5281/zenodo.20249312